

# REPORT

**Study Title:**

**DETERMINATION OF THE VAPOUR PRESSURE  
OF WACKER BS 1701**

**Data Requirement / Test Guidelines**

OECD No. 104, July 27, 1995  
Directive 92/69/EEC, A.4

**Study Director:**

Mrs. Alessandra Tognucci

**Study Completion Date:**

March 02, 2001

**Test Facility:**

**RCC Ltd**  
Environmental Chemistry &  
Pharmanalytics Division  
CH- 4452 Itingen/Switzerland

**Sponsor:**

**Wacker-Chemie GmbH**  
Johannes-Hess-Strasse 24  
D-84489 Burghausen/Germany

**RCC Study Number:**

797231



# GLP CERTIFICATE

The Swiss GLP Monitoring Authorities



Swiss Federal  
Office of  
Public Health



Swiss Agency for the  
Environment, Forests  
and Landscape



Intercantonal Office  
for the Control of  
Medicines

## Statement of GLP Compliance

It is hereby confirmed that

during the period of

August 15 – 17, 2000

the following Test Facilities of

**RCC Ltd**  
**4452 Itingen**  
**Switzerland**

were inspected by the Federal Office of Public Health, the Swiss Agency for the Environment, Forests and Landscape and the Intercantonal Office for the Control of Medicines with respect to the compliance with the Swiss legislation on Good Laboratory Practice.

### Test Facilities

### areas of expertise\*

- Toxicology Division

TOX, ACC

- Environmental Chemistry and  
Pharmanalytics Division

ACC, ECT, ENF, PCT, RES,  
OTH (Animal metabolism)

- Microbiological Diagnostics by  
Biotechnology & Animal Breeding Division

OTH (Microbiology)

The inspection was performed in agreement with the OECD Guidelines for National GLP Inspections and Audits. It was found that the aforementioned test facilities were operating in compliance with the Swiss Ordinance relating to Good Laboratory Practice [RS 813.016.5] at the time they were inspected.

Federal Office of Public Health  
The Director

Bern, November 2000

Prof. Th. Zeltner

\* TOX = Toxicology ; ACC = Analytical and Clinical Chemistry ; ECT = Environmental toxicity on aquatic and terrestrial organisms ; ENF = Behaviour in water, soil and air. Bioaccumulation ; PCT = Physical-chemical testing ; RES = Residue studies ; OTH = Other, to be specified.

## GOOD LABORATORY PRACTICE

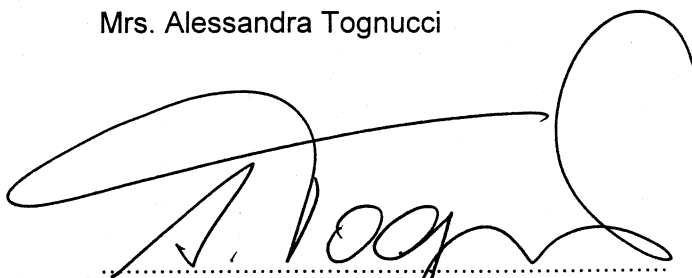
# STATEMENT OF COMPLIANCE

RCC Study Number: 797231  
Test Item: WACKER BS 1701  
Study Director: Mrs. Alessandra Tognucci  
Title: Determination of the Vapour Pressure of WACKER BS 1701

This study was conducted in compliance with the Swiss Ordinance relating to Good Laboratory Practice, adopted February 2<sup>nd</sup>, 2000 [RS 813.016.5]. This Ordinance is based on the OECD Principles of Good Laboratory Practice, as revised in 1997 and adopted November 26<sup>th</sup>, 1997 by decision of the OECD Council [C(97)186/Final].

There were no circumstances that may have affected the quality or integrity of the data.

Study Director: Mrs. Alessandra Tognucci

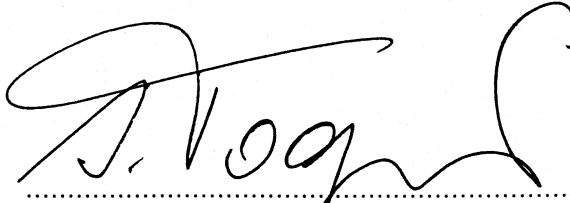


Date: March 02, 2001

## SIGNATURES

Study Director:

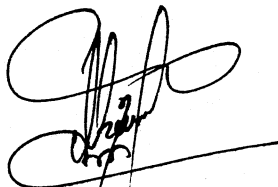
Mrs. Alessandra Tognucci

A large, stylized handwritten signature in black ink, appearing to read 'A. Tognucci', written over a horizontal dotted line.

Date: *March 02, 2001*

Management:

*h* Mr. Markus Arenz

A handwritten signature in black ink, appearing to read 'M. Arenz', written over a horizontal dotted line.

Date: *March 02, 2001*

## QUALITY ASSURANCE UNIT

RCC Ltd, Environmental Chemistry & Pharamanalytics Division, CH-4452 Itingen / Switzerland

### STATEMENT

RCC Study Number: 797231  
Test Item: WACKER BS 1701  
Study Director: Mrs. Alessandra Tognucci  
Title: Determination of the Vapour Pressure of  
WACKER BS 1701

The general facilities and activities are inspected periodically and the results are reported to the responsible person and management.

Study procedures were periodically inspected. The study plan and this report were audited by the Quality Assurance Unit. The dates are given below:

Dates and Types of QAU Inspections		Dates of Reports to the Study Director and to Management
December 27, 2000	Study Plan	December 27, 2000
January 05, 2001	Sample preparation; Measurement	January 11, 2001
February 17, 2001	Final report	February 17, 2001

This statement also confirms that this final report reflects the raw data.

Quality Assurance: Mrs. Ursula Memmert

Date:

*Ursula Memmert*  
March 02, 2001

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## PREFACE

### GENERAL

Title: Determination of the Vapour Pressure of  
WACKER BS 1701

Sponsor: Wacker-Chemie GmbH  
Johannes-Hess-Strasse 24  
D-84489 Burghausen/Germany

Study Monitor: Dr. Claus-Rüdiger Heikenwälder

Test Facility: RCC Ltd  
Environmental Chemistry & Pharamanalytics Division  
Zelgliweg 1  
CH-4452 Itingen / Switzerland

### RESPONSIBILITIES

Study Director: Mrs. Alessandra Tognucci

Deputy Study Director: Dr. Ute Schmiedel

Technical Coordinator: Mrs. Judith Frei

Head of RCC Quality Assurance: Mrs. Iris Wüthrich

### SCHEDULE

Experimental starting date: January 05, 2001

Experimental completion date: January 08, 2001

Date of report: March 02, 2001

### ARCHIVING

RCC Ltd, CH-4452 Itingen/Switzerland will retain the study plan, raw data, a sample of test item and the final report of the present study for at least ten years.

No data will be discarded without the sponsor's consent.

## **GUIDELINES**

This study followed the procedures indicated by the following internationally accepted guidelines and recommendations:

OECD Guideline for Testing of Chemicals No. 104: "Vapour Pressure", adopted July 27, 1995.

Directive 92/69/EEC, A.4, Vapour pressure, 1.4.1. Dynamic Method.

## **SUMMARY OF STUDY PLAN AMENDMENTS**

There were no amendments to the study plan.

# 1 PURPOSE

The purpose of this study was to determine the vapour pressure of WACKER BS 1701 by applying the dynamic method, which is suitable in the range of  $10^3$  Pa and  $10^5$  Pa. In the dynamic method, the boiling temperature, which pertains to a specified pressure was measured.

## 2 MATERIAL AND METHODS

### 2.1 TEST ITEM

Data as provided by the sponsor.

Identity:	WACKER BS 1701
Batch:	WF 85421
Purity:	94.54 %
Appearance:	Liquid, colourless
Expiration date:	December 01, 2002
Storage:	At room temperature (at approx. 20 °C)

### 2.2 REAGENTS AND TEST SYSTEM

No reagents were used to perform the study. The distillation apparatus was used during the laboratory part. A test vessel for the sample connected to a vacuum line and a system to regulate the pressure was used.

## 2.3 PRINCIPLE OF THE TEST

In this study the dynamic method was used to determine the vapour pressure of the test item as described in the Guidelines. The recommended range is  $10^3$  to  $10^5$  Pa. Preliminary, the vapour pressure of WACKER BS 1701 was calculated using the modified Watson Correlation [1]. The calculated value was 3.2 Pa at 25 °C. (Details are not reported here but are part of the raw data). Therefore the dynamic method was used for the determination of the vapour pressure of WACKER BS 1701.

### 2.3.1 Performance of the Test

The test item was filled in a 250 ml three-necked glass flask equipped with a magnetic stirrer, reflux condenser and a thermometer. The thermometer reached into the space between the test item and the lower part of the reflux condenser. The upper part of the condenser was connected to a vacuum pump with adjustable pressure. To avoid overheating the content of the flask was stirred magnetically. The vacuum pump produces pressures between about 10 mbar and 230 mbar (which is equal to 1000 Pa - 23000 Pa) in the system. The apparatus was heated using a temperature controlled oil bath.

The pressure was changed and the corresponding boiling temperature measured.

The main test was carried out three times. During each main test at least 10 values were measured. The heating was stopped at 181 °C in the first main test, at 180 °C at the second test and at 179 °C in the third test. Details of the measured values are given in Table 1 to 3.

## 2.4 DATA HANDLING

The vapour pressure of WACKER BS 1701 was calculated using the measured boiling temperatures with the respective pressure values. The boiling temperatures in 1/K are plotted against the corresponding pressures as  $\ln P_{vp}$ . A correlation of these values was prepared. The vapour pressure of WACKER BS 1701 was extrapolated to 25 °C using these values. The extrapolated pressure at 25 °C is equal to the vapour pressure at this temperature.

This curve was used for the extrapolation of the vapour pressure of WACKER BS 1701 at 25 °C.

$$Y = b \cdot x + a$$

where

- Y =  $\ln P_{vp}$  (measured pressure)
- x =  $1/T$  (K) (measured temperature in Kelvin)
- b = slope
- a = y-axis intercept

[1] W.J. Lyman, W.F. Reehl and D.H. Rosenblatt (ed.), Handbook of Chemical Property Estimation Methods, McGraw-Hill, NY (1990).

### 3 RESULTS

The determination of the vapour pressure of WACKER BS 1701 was performed according to the EEC Directive 92/69, A.4 "Vapour Pressure" (1992) and the OECD guideline No. 104, "Vapour Pressure" (1995) using the dynamic method.

Preliminary, the vapour pressure was calculated to be 3.2 Pa at 25 °C using the modified Watson correlation.

During the tests, the boiling temperature and the respective vapour pressure was measured. The individual values of the three tests and the extrapolation data are summarised in Table 1 to 3. Based on the experimental results the vapour pressure curve  $\ln P_{vp}$  versus  $1/T$  was plotted (see Figure 1 to 3). The vapour pressure of WACKER BS 1701 at 25 °C was extrapolated from the determined values for each test.

The extrapolated vapour pressure of the first experiment was  $1.11 \times 10^{-1}$  mbar which is equal to 11.1 Pa at 25 °C. The second test indicates a vapour pressure at 25 °C of  $7.83 \times 10^{-2}$  mbar which is equal to 7.83 Pa. During the third test a vapour pressure at 25 °C of  $8.02 \times 10^{-2}$  mbar which is equal to 8.02 Pa was measured.

In conclusion, the vapour pressure of WACKER BS 1701 was determined to be

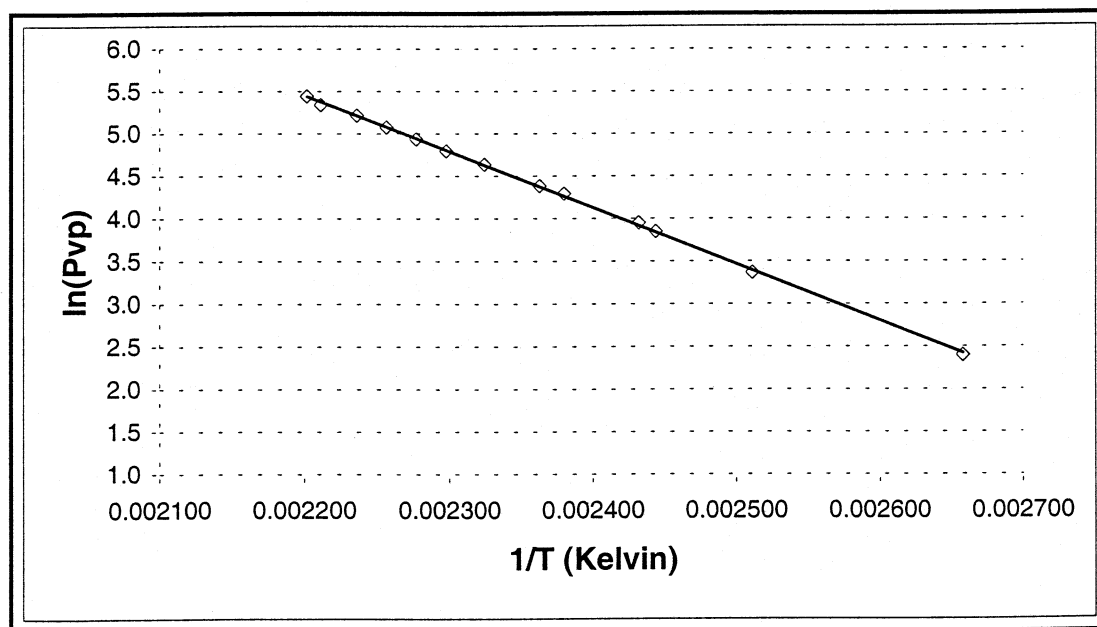
**9.0 Pa at 25 °C**

using the dynamic method.

Table 1: Determination of boiling points at reduced pressures and the extrapolation data (1. experiment)

Boiling temperature (°C)	Pressure measured (mbar)	1/T (Kelvin)	ln Pvp
103.0	11.0	0.002658	2.4
125.0	29.0	0.002511	3.4
136.0	47.0	0.002444	3.9
138.0	52.0	0.002432	4.0
147.0	73.0	0.002380	4.3
150.0	80.0	0.002363	4.4
157.0	103.0	0.002325	4.6
162.0	121.0	0.002298	4.8
166.0	139.0	0.002277	4.9
170.0	160.0	0.002256	5.1
174.0	184.0	0.002236	5.2
179.0	209.0	0.002211	5.3
181.0	231.0	0.002202	5.4

Figure 1: Extrapolation of the Vapour Pressure of WACKER BS 1701 (1. experiment)



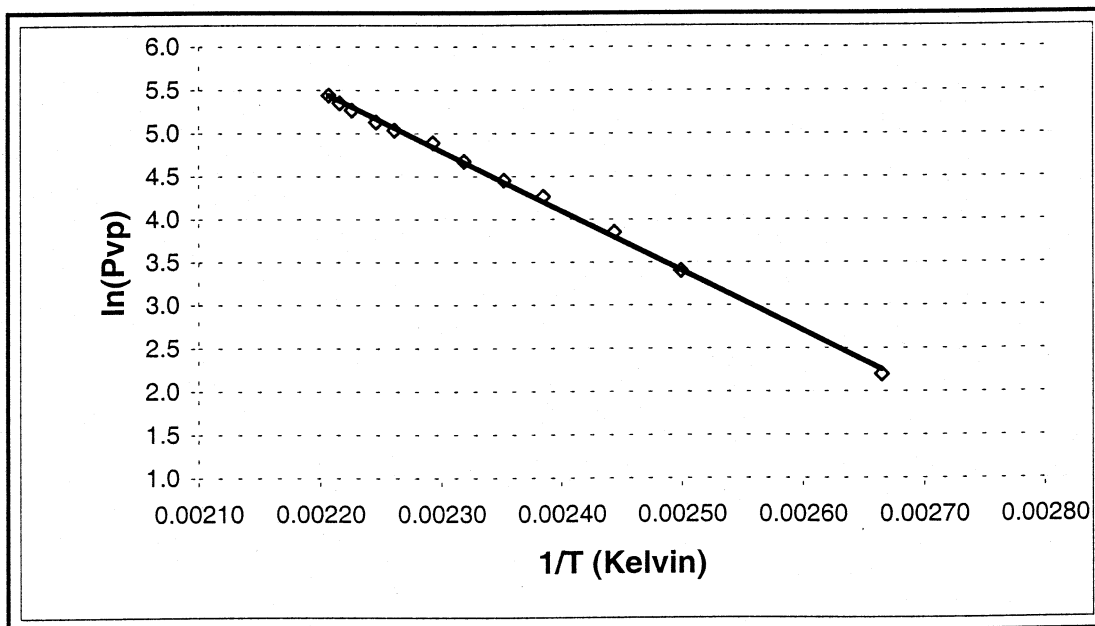
$$Y = b \cdot x + a \quad \text{with} \quad \begin{aligned} Y &= \ln P_{vp} \text{ (} P_{vp} \text{ in mbar/hPa)} \\ x &= 1/T \text{ (Kelvin)} \\ b &= -6618.9 \quad \text{(slope)} \\ a &= 20.01 \quad \text{(y-axis intercept)} \\ r^2 &= 0.9995 \end{aligned}$$

Extrapolated vapour Pressure: 11.1 Pa at 25 °C.

Table 2: Determination of boiling points at reduced pressures and the extrapolation data (2. experiment)

Boiling temperature (°C)	Pressure measured (mbar)	1/T (Kelvin)	ln Pvp
102.0	9.0	0.002665	2.2
127.0	30.0	0.002499	3.4
136.0	47.0	0.002444	3.9
146.0	71.0	0.002385	4.3
152.0	86.0	0.002352	4.5
158.0	107.0	0.002319	4.7
163.0	133.0	0.002293	4.9
169.0	154.0	0.002261	5.0
172.0	169.0	0.002246	5.1
176.0	194.0	0.002226	5.3
178.0	211.0	0.002216	5.4
180.0	230.0	0.002207	5.4

Figure 2: Extrapolation of the Vapour Pressure of WACKER BS 1701 (2. experiment)



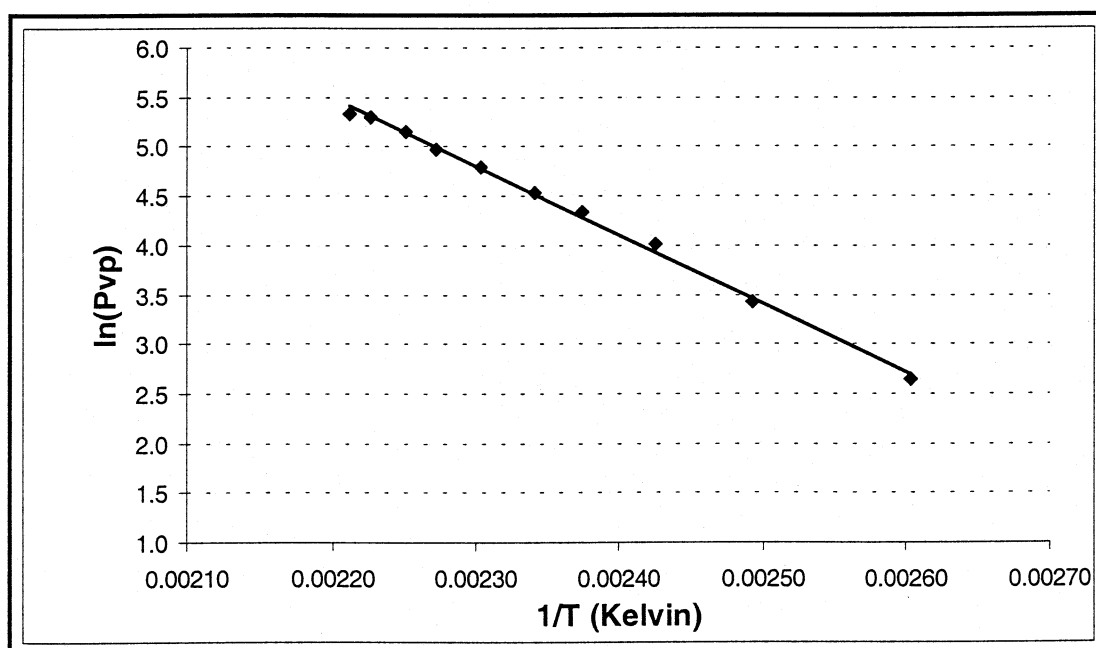
$$Y = b \cdot x + a \quad \text{with} \quad \begin{aligned} Y &= \ln P_{vp} \text{ (} P_{vp} \text{ in mbar/hPa)} \\ x &= 1/T \text{ (Kelvin)} \\ b &= -6952.9 \quad (\text{slope}) \\ a &= 20.785 \quad (\text{y-axis intercept}) \\ r^2 &= 0.9982 \end{aligned}$$

Extrapolated vapour Pressure: 7.83 Pa at 25 °C.

Table 3: Determination of boiling points at reduced pressures and the extrapolation data (3. experiment)

Boiling temperature (°C)	Pressure measured (mbar)	1/T (Kelvin)	ln Pvp
111.0	14.0	0.002603	2.6
128.0	31.0	0.002493	3.4
139.0	55.0	0.002426	4.0
148.0	76.0	0.002374	4.3
154.0	93.0	0.002341	4.5
161.0	121.0	0.002303	4.8
167.0	145.0	0.002272	5.0
171.0	173.0	0.002251	5.2
176.0	200.0	0.002226	5.3
179.0	219.0	0.002211	5.4

Figure 3: Extrapolation of the Vapour Pressure of WACKER BS 1701 (3. experiment)



$$Y = b \cdot x + a \quad \text{with} \quad \begin{aligned} Y &= \ln P_{vp} \text{ (} P_{vp} \text{ in mbar/hPa)} \\ x &= 1/T \text{ (Kelvin)} \\ b &= -6934.9 \quad \text{(slope)} \\ a &= 20.758 \quad \text{(y-axis intercept)} \\ r^2 &= 0.9971 \end{aligned}$$

Extrapolated vapour Pressure: 8.02 Pa at 25 °C.